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Design of a silicon nitride mirror for constructing a high Quality cavity for coupling to Rubidium-87 atoms

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Abstract

In order to investigate light-matter coupling, a cavity is required with a high Q-factor to support the modes for a certain wavelength. Here, we construct a mirror out of a silicon nitride (SI₃N₄) ridgewaveguide, which has a refractive index of n = 2. The mirror may then be used to construct a cavity. The mirror has a height h = 200nm. Since the cavity will be used in experiments with Rubidium-87 atoms, the goal is to obtain a mirror with a band gap centred at $\lambda = 780$ nm, where λ denotes the wavelength. For the design of the mirror finitediference time-domain (FDTD) simulations are performed to investigate the effect of individual structural components on the band gap. With the results obtained from these FDTD simulations we designed a mirror with a band gap centred at $\lambda = 780$ nm while keeping scattering losses in the order of 10^{-3} . By extending the mirror size we show that these losses even have the potential to be reduced further by one order of magnitude, i.e. 10^{-4} .

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1 Introduction

Since even before the discovery of the atom, light-matter interactions where a fascinating subject in physics. Interactions such as the photoelectric effect are at the basis of quantum mechanics[1] which is one of the most successful theories in modern physics.

More recently a different kind of interaction has caught the attention of researchers and engineers alike. The light matter coupling is a regime within which confined photonic modes and excitation states of matter are coupled[2]. The investigation of a single atom interacting with a single electromagnetic field mode is the main subject of cavity quantum electrodynamics (QED)[3].

Currently there is a lot of research in the field of cavity QED[2,4,5]. In fact the awarded noble Prize in physics of 2012 was related to this field[6]. Revolutionary developments such as quantum information processing[7] as well as the design for tools such as the nanocavity lasers[8,9] rely on these interactions.

An important factor to achieve coupling is off course the confinement of the modes in a cavity[10]. So the realisation of a system that contains such cavity is essential to the coupling process. The origin of these optical cavities are defects in the structure of photonic crystals. Yet the use of crystals such as the multilayer film[10] is unpractical. The fabrication methods[11,12] make the implementation of a defect and the dictation of the structural size challenging.

Fortunately there are alternative designs[13,14]. The most applied one is made out of a ridge-waveguide with an array of cylindrical air holes drilled periodically into them. The cavity here is a spacing between two holes that is larger than the separation of the other holes. This introduces a defect in otherwise a periodic system. The holes on either side of the defect act as frequency specific mirrors effectively creating a band gap[10]. Because the periodicity of the system is along one direction, the defect is known as a one dimensional cavity.

There is a great focus on designing cavities of this structure with ultra high Q factors[4,15]. The quality of the cavity, that is to say the rate of energy loss, is given by this Q factor. Ultimately one wants a cavity with a high Q factor to promote light mater coupling. As neatly demonstrated by McCutcheon and Lončar for a one dimensional construction, the quality of the cavity can significantly improve when a taper is introduced in the design. The tapers job is to smooth over the transition of the effective index between the cavity and the mirror to prevent scattering. This results to a better reflection on the mirrors part and thus a higher Q factor for the cavity.

A great feature of this design is the relative ease with which the system

can be realised and customised in comparison to multilayer film. There is however a drawback. Whereas the cavity modes of a multilayer structure have an analytically solution[10], the modes in this model do not. One has to resort to simulations to find these modes before the actual construction of the cavity.

McCutcheon and Lončar intend to use their cavity to realise a coupling with the nitrogen-vacancy in a diamond nano-crystal. This requires them to centre the band gap of their mirror at a 637 nm wavelength[4]. The research group I am working with is interested in a high quality cavity that supports coupling to Rubidium-87 atoms. The band gap for this cavity has to be at 780 nm. Normally, by the scale invariance of the Maxwell equations[10], an easy rescaling of McCutcheon and Lončar design would provide the required band gap. However the strips used to make these cavity structures are cut out of a plate of silicon nitride. The plates available to us have a thickness of 200 nm which is about 44 nm short of what is required.

The subject of this thesis is then to find an alternative construction of the same design that provides us with a band-gap centered at 780 nm while keeping the height below 200 nm. To be more specific, we are looking for the width and the height of the wave guide along with the radius and separation of the holes. In the process of doing so, we will also investigate the effect of structural components on the band-gap and scattering loss. These may then be used for optimisation and gap-relocation purposes.

Once the mirror structure is specified and optimised one can use it to find the cavity that supports the required modes. Note that the two sides of the cavity are symmetric and therefore finding one will suffice. The system as a whole can be optimised again to improve the quality of the cavity.

2 Theory

The design that we are interested in is of a cavity in a periodic dielectric waveguide. The concept of a cavity however, is much easier explained in terms of a defect in a multilayer film. So we will start by explaining the basic concept of a photonic crystal. After that we write down the Maxwell equations and derive them to a more appropriate form. In subsection 2.2 the multilayer model will be used to explain band-gaps and eventually cavities. Finally we will compare the multilayer model with the periodic dielectric waveguide and discuss how the shared properties can be used to support localised modes in the cavity of the waveguide.

Most of the explanations in this section are conceptual and there are no

explicit calculations. Moreover, the details are kept to those necessary for the understanding of band-gaps.

2.1 Photonic Crystal and the Maxwell equations.



Figure 1: Examples of one- two- and three dimensional photonic crystals. The different colours represent materials with different dielectric constants. Image from [10].

Much like the solid crystalline, the photonic crystal has repeating structure. The pattern consists of altering dielectric constants. This pattern repeats itself along one, two or three axes which correspond to a one-, two- or three dimensional photonic crystal as displayed in figure 1. Mathematically the structure can be described with a function of the dielectric constant[10]. In three dimension this function takes the form $\epsilon(\mathbf{r})$.

The main difference between atomic and photonic crystals are their respective length scales. The solid crystalline has a repeating structure of atoms whereas the photonic crystal repeats itself at a macroscopic scale. This difference also dictates the scale on which the two crystals are applied. For instance, some atomic crystals may be used for scatter electrons[16,17]. In crystallography[18] however electron scattering is used to study the crystals structure. What ever the case may be, the de Broglie wavelengths of the scatted electrons are in the pm (10^{-12}) range whereas the photonic crystal operate in the nm (10^{-9}) range.

Indeed the main use of photonic crystals involves reflection and scattering of light. Since light is an electromagnetic wave its properties are governed by the Maxwell equations[10].

$$\nabla \cdot \mathbf{B} = 0, \quad \nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0,$$

$$\nabla \cdot \mathbf{D} = \rho, \quad \nabla \times \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} = \mathbf{J}.$$
 (2.1)

Where **E** is the electric field, **H** the magnetic field, **D** the displacement field and **B** the induction field. ρ and **J** are the free charge and current density respectively. These two will be set to zero since we are considering crystals that are not charged and do not have a current running trough them.

Now we relate **D** to **E** via a power series

$$\frac{D_i}{\epsilon_0} = \sum_j \epsilon_{ij} E_j + \sum_{j,k} \chi_{ijk} E_j E_k + O(E^3)$$
(2.2)

This equation relates the D_i component of the Displacement field to the E_i component of the electric field. Where $\epsilon_0 \approx 8.854 \times 10^{-12}$ F/m is the permittivity of vacuum. Note that a similar equation can be written to relate **B** to **H**[10].

For many dielectrics it is reasonable to make some approximations[10]. First assumption is that the field strength in the crystal is small enough to ignore all but the linear terms on the right hand side of Equation 2.2. Also you can assume that the medium is macroscopic and isotropic. In that case **E** and **D** are related by the dielectric function $\epsilon(\mathbf{r}, \omega)$ multiplied by the permittivity of vacuum. The function $\epsilon(\mathbf{r}, \omega)$ is known as the relative permittivity. Further approximation can be made by ignoring material dispersion. Instead one just chooses a dielectric constant appropriate for the size of the system under consideration. We will also only consider transparent mediums and so the relative permittivity is real and positive.

To the system we are considering all these approximations are applicable and so we may proceed to get[10]:

$$\mathbf{D}(\mathbf{r}) = \epsilon_0 \epsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}), \quad \mathbf{B}(\mathbf{r}) = \mu_0 \mu(\mathbf{r}) \mathbf{H}(\mathbf{r}). \tag{2.3}$$

Where $\mu_0 = 4\pi \times 10^{-7}$ H/m is the permeability of vacuum. But for the most dialectics of interest μ will be close to 1 so we may omit it from the equation above that relates to **B**(**r**). In that case the relative permittivity becomes the square of the refraction index. Now we can rewrite the Maxwell equations as:

$$\nabla \times \mathbf{E}(\mathbf{r}, t) + \frac{\partial \mathbf{B}(\mathbf{r}, t)}{\partial t} = 0, \quad \nabla \times \mathbf{H}(\mathbf{r}, t) - \frac{\partial \mathbf{D}(\mathbf{r}, t)}{\partial t} = 0, \quad (2.4)$$
$$\nabla \cdot \mathbf{D}(\mathbf{r}, t) = 0, \quad \nabla \cdot \mathbf{B}(\mathbf{r}, t) = 0.$$

Because the Maxwell equations are linear we can separate the time dependence from the spatial dependence and express the fields as harmonic modes[10]. Since all functions can be expressed in a set harmonic modes, this wont limit our fields. Furthermore, for mathematical convenience we will write the fields down as complex functions of spatial pattern multiplied my a complex exponential and take the real part for physical fields.

$$\mathbf{H}(\mathbf{r},t) = \mathbf{H}(\mathbf{r})e^{i\omega t}, \quad \mathbf{E}(\mathbf{r},t) = \mathbf{E}(\mathbf{r})e^{i\omega t}.$$
(2.5)

Putting Equations 2.5 in the divergence Equations of 2.4 gives us the requirement that the waves are transverse[10], which is a known fact for light waves. The two Equation in 2.4 that involve the curl of the fields can be used to relates \mathbf{E} to \mathbf{H} . Using all this we get:

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) - \epsilon(\mathbf{r})k_0^2 \mathbf{E} = 0,$$

$$\nabla \times \frac{1}{\epsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) - k_0^2 \mathbf{H} = 0$$
(2.6)

with $k_0^2 = \epsilon_0 \mu_0 \omega^2$.

Solving Equation 2.6 for a given structure $\epsilon(\mathbf{r})$ provides an analytic solutions for the modes[10]. The modes of the electrical field are solved by the equation involving $\mathbf{E}(\mathbf{r})$ and that of the magnetic field by the one involving $\mathbf{H}(\mathbf{r})$. However it is customary to only solve the modes of the magnetic field. The electric field can than be taken trough the relation between the two fields. Yet this has to do with mathematical convenience and in principle both Equations can be solved separately.

Note that equation 2.6 is scale invariant. If we were to rescale the structure of the crystal by some scalar constant, then the modes and there frequencies will scale accordingly but equation 2.6 will stay the same. Therefore if you find the solution at one length scale you have found them at all macroscopic length scales. This is known as the scale invariance of the Maxwell equations[19].

2.2 One dimensional crystal and photonic band-gaps

A one dimensional crystal can be represented by a multilayer film with altering permittivity along a single axis. An image is shown in figure 2. Such an object can mathematical be described by

 $\epsilon(z+Z) = \epsilon(z)$

Taking the z-axis to be perpendicular to the film layers and Z any integer multiple of the spatial periodicity a. This indicates a displacement symmetry with a displacement vector Z in the direction of z.

Within a periodic structure the modes that makes up the wave functions take the form[10]

$$\mathbf{H}_{nk_z\mathbf{k}_{||}}(\mathbf{r}) = e^{i\mathbf{k}_{||}\cdot\mathbf{p}} e^{ik_z z} \mathbf{u}_{nk_z\mathbf{k}_{||}}(z).$$
(2.7)



Figure 2: The multilayer film consisting of alternating layers of materials with different dielectric constants. The crystal extends to infinity in all directions. Image from [10].

This is known as the Bloch form with n the nth eigenstate or mode of the field which corresponds to the nth eigenvalue of frequency ω_n . The wave vector \mathbf{k} is divided in \mathbf{k}_{\parallel} that contains the components parallel to the films and k_z is the z component. Also \mathbf{p} is parallel to the film and $\mathbf{u}(z)$ is a periodic function with periodicity a. Note that we didn't write down the eigenstates of the electrical field. However both fields can be written in this form. Moreover the fields are related and can easily be converted into one another. Equation 2.7 is known as TM-modes and the electric counter parts are called TE-modes[10].

For a crystal that is big in comparison to the size of modes and therefore can be considered as infinitely large, the continuous translation symmetry allows for $\mathbf{k}_{||}$ to take any value. On the other hand k_z may be restricted to a finite interval due to the discrete translation symmetry of the crystal along the z axis. For now lets consider the case that $\mathbf{k}_{||}$ is zero. This will leave us with a wave which is parallel to the film layers and is propagating in the z direction only. Looking at Equation 2.7 we see that the exponential with the $\mathbf{k}_{||}$ argument becomes equal to one and thus vanishes from the Equation. The remainder is a product of two periodic functions in z that have a periodic dependence on a. More specifically, there is no physical difference between the Bloch states with wave vector k_z and wave vector $k_z + 2\pi m/a$, with m any integer constant. The mode frequency is off course also the same. For this reason we only consider k_z in an interval of $[-\pi/a, \pi/a]$. this is known as the Brillouin zone[20].

At the border of these Brillouin zones were $k_z = \pi/a$ the modes have a wave length of 2*a*. In order to maintain symmetry of the unit cell about its centre, the mode can take only two configurations[10]. One is having its node at the centre of the low ϵ and the other is at the centre of the high ϵ medium. As can be seen figure 3 (a) and (b). These two separate configurations, although having the same wavelength, are not the same. They are in fact two different modes. There is a clear difference in the distribution of energy over the unit cell between the two modes as shown in figure 3 (c) and (d).

In general, low frequency modes concentrate there energies in high ϵ regions while high frequencies tend to have large fraction of there energies in the low ϵ regions[10]. This effectively creates a gap in possible frequencies that the modes can have. This is known as the photonic band gap[14]. A similar feature occurs in solid state physics where the electron state can not exist in a certain energy region[21]. This energy gap is confined between the valance band and the conducting band of an insulator or a semiconductor. Anyways, the size of the photonic band gap depends greatly on the contras of permittivity within the crystal. This size is often expressed as the ratio of the width and central frequency of the gap. This is the so called gap-midgap ratio[10].

With regards to the off-axis propagation, all that we need to know is that there is no band gap in the directions where there is no spatial periodicity[10]. The details of this are not relevant to our goal and so we will proceed without discussing them.

So far we have only considered perfect infinite size crystals. However some interesting and useful properties are obtained by creating a crystals with a defect in its structure. First lets take a one dimensional crystal that has a finite size in the periodic direction. We can now send a pulse of light with a range of frequencies through the surface of the crystal. As before we are considering plane waves that are propagating in the z-direction (onaxis propagation). As the pulse enters the crystal the modes outside of the band gap will extend trough the crystal and are therefore called the extended modes. The modes that have their frequencies in the band gap will decay exponentially. The closer the modes are to the centre of the gap the faster they will decay. These are known as the evanescent states[10].

Now suppose that we have an otherwise perfect crystal except for layer of film that has a different width than the rest. A sketch is shown in figure 4. Far from this defect we expect the crystal to behave as a perfect crystal. However in the vicinity of the defect, symmetry is clearly broken and that may lead to localisation of modes in that region. In general the system can been seen as two perfect crystals lined up and between them is the defect layer also known as the cavity. Modes trapped inside the cavity will just bounce back and forth. The two sides act as frequencies specific mirrors.



Figure 3: (a) The lowest TE-mode band 1; (b) the highest TE-mode of band 2; (c) electric field energy density of the lowest TE mode of band 1; (d) electric field energy density of the highest mode of band 2. Where band 1 is under the band gap and band 2 is above the band gap. Image from [10].

This may lead to the quantisation of the modes to discrete frequency that lie in the perfect crystals band gap. A state density graph is sketched in figure 5. These modes are known as localised modes[10].



Figure 4: A on dimensional crystal with a defect layer. Image from [10].



Figure 5: A plot of the density of state as a function of frequency inside the cavity. The mode labelled as the defect state is a localised mode . Image from [10].

2.3 Periodic waveguide

In the previous subsection I discussed the properties of the multilayer film. We intend to use the periodic dielectric waveguide as an alternative design to the multilayer film. This is off course only possible it the two models share the necessary properties. In this subsection we discuss these properties and show how they are shared by both systems. First consider the 3 dimensional waveguide[22] without the cylindrical holes. This is basically a long dielectric medium. Given that the medium has a larger index than its surroundings, total internal reflection will provide waves that propagate closely along the long axis of the waveguide.

Adding the holes, the system gains a periodicity along the long axis. This periodic dielectric waveguide[22] resembles the one dimensional photonic crystal in that it has discreet translational symmetry along its long axis. Much like in the multilayer film, this symmetry will lead to extended modes and photonic band-gaps[10]. Figure 6 shows the two modes at edge of the Brilluoin zone for the periodic waveguide. This is equivalent to Figure 3 where the modes at the edge of the Brilluoin zone for the multilayer film were shown.



Figure 6: The two TE-modes at the edge of the Brilluoin zone. The left image shows the mode just under the gap. The right image shows the mode just above the gap. Image from [10].

Consider now the periodic dielectric waveguide with a cavity[14] somewhere in the middle of its structure. This off course disturbs the periodicity just as the defect layer did for the multilayer film. When I discussed localised modes in the last Subsection, I mentioned that the two sides of the cavity in the multilayer film form a frequency specific mirror. The periodic waveguide does the same but suffers greatly from scattering losses. This limits the systems capability to support localised modes.

Fortunately we know this can be reduced significantly by using a taper[4]. Figure 7 shows the one dimensional cavity design for a periodic waveguide with the mirror and taper included. The taper is made from an array of holes with increasing radius and separation. The taper is placed between the cavity and the mirror to smooth the transition between the effective index of the cavity modes and the mirror. Using the structure of Figure 7 we can create cavity modes similar to the localised modes in the defect of the multilayer film.

It turns out that the periodic dielectric waveguide provides everything



Figure 7: The structure of a cavity made out of a dielectric waveguide.

necessary to construct cavities. The challenge now is to use this design to find a cavity with a high Q-factor that supports specific modes. Usually this is done using simulation software since there is no analytic solution to the structure.

3 Simulations and FDTD

3.1 Simulations

To find the localised modes in the cavity of a periodic deictic waveguide, one has to resort to numerical methods. Fortunately one does not need to be a skilled programmer to apply them. There are user friendly software packages that have these methods implanted. So when familiar with the interface of the package, the modes can be found without any actual programming on the users part.

One such software package is the MIT electromagnetic equation propagation (Meep). The numerical method that Meep uses is the finite difference time domain (FDTD)[24,25,26]. The main use of this software package is the computing of transition, reflection and scattering spectra in addition to the resonant modes. These are the exact features that one needs to find the band gap and cavity modes of the system considered in this thesis.

While there is no need to program the method yourself, it is always a good idea to understand the scheme on a mathematical level. This will help determining accuracy and is neccessry to explain unexpected deviations if they are due to the numerical method. Therefore the next subsection is a bief introduction to the FDTD method.

3.2 FDTD

As the names suggests, the FDTD belongs to the class of grid-based finite difference methods. These methods are used to find approximate solutions to differential equations [26]. This comes down to replacing the derivatives by a finite difference equations. It is also a time domain method which

basically takes the Maxwell Equations and evolves them over time in a finite computational region. So the FDTD approximates both the spatial and the time derivatives[24] in the Maxwell Equation by finite differences. In one dimension this approximation can be derived by Taylor expanding a function around a point x_0 with a small offset $\frac{\delta}{2}$. Actually the function is expand twice, once with a positive and once with a negative offset.

$$f(x_0 + \frac{\delta}{2}) = f(x_0) + \frac{\delta}{2}f'(x_0) + \frac{\delta}{2!}f'(x_0)' + \frac{\delta}{3!}f'''(x_0)...,$$

$$f(x_0 - \frac{\delta}{2}) = f(x_0) - \frac{\delta}{2}f'(x_0) + \frac{\delta}{2!}f'(x_0)' - \frac{\delta}{3!}f'''(x_0)....$$
(3.1)

where the number of primes indicate the degree of the derivatives. By subtracting the second by the firs Equation and dividing by δ we get:

$$\frac{f(x_0 + \frac{\delta}{2}) - f(x_0 - \frac{\delta}{2})}{\delta} = f'(x_0) + \frac{\delta^2}{2 * 3!} f'''(x_0)....$$
(3.2)

The first term on the right is just the first derivative of f at x_0 . All the other terms on the right side are the higher derivatives at x_0 multiplied with δ of order 2 and higher. When all these higher derivatives are summed up and Equation 9 is rearranged we can write down the identity as

$$\frac{df(x)}{dx}\Big|_{x=x_0} = \frac{f(x+\frac{\delta}{2}) - f(x-\frac{\delta}{2})}{\delta} + \sigma(\delta^2)$$
(3.3)

where σ denotes the infinite sum of higher derivatives. Note that this sum get smaller with δ . At the limit both δ and σ go to zero. In that case we just get the definition of the derivative. When δ is taken to be sufficiently small we can thus approximate the derivative by[24]

$$\frac{df(x)}{dx}\Big|_{x=x_0} \approx \frac{f(x+\frac{\delta}{2}) - f(x-\frac{\delta}{2})}{\delta}$$
(3.4)

This is known as central difference, as you approach x_0 from both sides. A similar approximation can be made by approaching x_0 from the left or the right. These are known as forward and backward difference respectively. Higher derivatives can be approximated by similar fashion.

Notice the term σ that was ignored is in fact the error of the approximation. It gives an indication to the relative improvement as δ gets smaller. Loosely speaking, if you reduce the δ by a factor of 10 the error will reduce by a factor of 100. This is off course due to the lowest order of δ in σ which was 2. Therefore this approximation is said to have a second order accuracy[26].

This concludes the introduction to FDTD. Yet there is still a lot to contemplate about before one decides to use a scheme for a particular system. Aspects as stability and suitability must be considered. Fortunately this has all been done for me. The software package (Meep) that I am using is specifically designed to model electromagnetic systems such as the one under consideration. Therefore I will proceed without considering these matters.

4 Simulations and results

4.1 Goal

In Subsection 2.3 a frequency specific mirror made out of a periodic dielectric waveguide was discussed. My goal is to find the specific structure of this mirror such that its centre-gap frequency has a wavelength of 780 nm while keeping loss by scattering to a minimum. By finding the specific structure I mean determining the width of the waveguide w, the height h, the radius of the cylindrical holes r and the centre to centre distance of the cylinders d. The general structure is shown in figure 8. The mirror is made out of SiN_x which has a refraction index of 2 and its height must not be larger than 200 nm.



Figure 8: The periodic dielectric mirror with a taper.

4.2 Simulation geometry

To find this specific structure I have used a simulation software that makes use of the finite-difference time-domain (FDTD) method. See section 3 for more details about FDTD simulations. The geometry of the simulated structure consist of the periodic waveguide as show in figure 8. Note that this image only shows the mirror and taper side of the system. In addition to this, there is a source at the opposite end of the waveguide. The part of the waveguide in between the taper and the source is roughly six times the size of the mirror. Furthermore, the light pulse must have an equal intensity in a specific range of frequencies. Either the source provides such pulse or one has to normalise it before making calculations. Also note that the simulated region has a width and height that is about five times the width of the waveguide. A perfect matched layer (PML), a fictional layer which absorbs the electromagnetic waves, forms the boundary of this region. However the waveguide starts at one side of the region and ends at the other side. One has to make sure that the source and the mirror are placed at a distance from the boundary so that they do not get covered by the PML.

4.3 Replication



Figure 9: The graph of McCutcheon and Lončar on 5 differnt design for the photonic crystal mirrors. Image from [4].

In a series of 5 simulation, McCutcheon and Lončar have shown the effect of taper size (number of holes) on the reflectivity of the mirror[4]. Their graph is shown in Figure 9. As the taper increases from zero to seven there is a clear and strong impact on the structure of the band-gap as whole. Not only does an increase in taper size decrease scattering, effectively increasing the Q factor, but also changes the centre wavelength of the band gap. This is explained as mismatch between the effective index of the Bloch modes and the effective index of the mirror[27]. The mismatch can be smooth over by changing the effective index gradually rather than suddenly. There is however no need to make the taper much bigger as the effect becomes insignificant once the transition is smooth enough.

We reproduced the results by McCutcheon et al. for a mirror with seven tapers. A graph of the band-gap can be seen in figure 10 and the dimensions



Figure 10: The band gap structure of the periodic dielectric mirror including the structural dimensions

of the waveguide are listed there as well. Note that the results are not identical as I choose a 7 hole mirror whereas they used 14 holes. Also the resolution they used for their simulations was not specified, yet I suspect their simulations to be at a higher resolution.

When more holes are added to the mirror a sort of oscillation forms in the structure of the band-gap. This will make an accurate determination of the minimum impossible. The issue can be solved using a higher resolution. Doubling the resolution however, results in 16 times the simulation time. Considering the processing power at my disposal, it will take 8 days of simulation time per set. This is the reason we limited the mirror size to 7 holes.

Despite all that, the structure and location of the band-gaps are in agreement. Both are centred around 635 nm wavelength and both have similar widths close to the centre of the gap. However its clear that one reflects better than the other. McCutcheon and Lončar reach a Loss as small as 10^{-3} whereas my system does not quite reach that quality. This is not surprising, they have after all used 7 more mirror holes than i did.

Nonetheless the agreements are good enough to proceed in this fashion. At this stage the main concern is the location of the band gap rather than its optimisation. Once we figure out how to relocate the band-gap, we can always add more holes to the mirror and increase resolution to get a better results.

4.4 Structural effects

In the last subsection a structure of the mirror was presented. A variation of each structural component individually from it, revealed their effects on the form and location of the band-gap. The results of a variation of a small fraction ($\approx 10\%$) to the radius and separation of the holes are shown in figure 11. It seems that the centre-gap wavelength is not very sensitive to a small change of these components. On the other hand the scattering is. Which leads to the conclusion that the radius and separation are better suited for optimisation of the mirror rather then the relocation of the band-gap.



Figure 11: A fractional variation of $\approx 10\%$ to the separation is shown in the left plot and to the radius in the right plot.

Variations regarding the height and width of the waveguide results in similar scattering issues with the very important distinction that the latter two do have a significant impact on the location of the band-gap. An increase in height or width of the waveguide will take the gap to larger wavelengths. The results will be presented with more detail in the next subsection.

It was expected that any change resulting in a higher effective index of the waveguide would lead to an increase of the gaps wavelength. Yet we did not know how much this increase would be or how it would effect scattering.

4.5 Rescaling

By the scale invariance of the Maxwell equations, one could rescale the mirror of presented in Subsection 4.3 to fit the desired band gap. This will however

result on a height of the structure larger than 200 nm. Fortunately, the effect of the structural components are known. Once the system is rescaled, the height can be decreased to its maximum value and the width can be increased to compensate. This will come at the expense of the mirrors efficiency but the loss can somewhat be confined by optimisation.

In figure 12 a graph of the gaps centre wavelength is shown as a function of the width. The corresponding loss is included as well. This is of the rescaled structure with the height at its maximum. The structural values can be seen in table 1.



Figure 12: The centre gap wavelength as a function of the width of the waveguide in addition to the corresponding loss shown on the right vertical axis.

This graph shows that a width of 450 nm will bring the centre-gap wavelength to a close proximity of 780 nm. Moreover, it does so without a significant increase in scattering. Also notable is the linearity in the increase of the wavelength which lead to a interesting feature. Consider rescaling the waveguide listed in Figure 10 to have its centre-gap wavelength at 780 nm without limiting the height. It turns out that this waveguide has almost the same cross-section area as the 200 by 450 nm waveguide. That is to say, both mirrors have there band gap centred at 780 nm wavelength and also have nearly the same cross-section area.

This hints towards a relationship between the cross-section area and the

location of the band-gap. This relationship must naturally include the cylindrical holes somehow. So it is most likely that the relationship involves the effective index rather than cross-section area. This was of course expected as noted earlier. Note however that if this is true, then the linearity in the increase of the wavelength is going to break down at large widths. In the limit of the width going to infinity, the effective index is just going to reach the index of a homogeneous medium made out of nitrogen silicon.

Width waveguide	270 to 450 nm
Height waveguide	200 nm
Mirror size	7 holes
Mirror radius	84 nm
Mirror separation	300 nm
Taper size	7 holes
Taper radius	66 to 84 nm
Taper separation	257 to 300 nm

Table 1: The structural dimensions of the dielectric waveguide mirror.

4.6 **Optimisation**

With the width set at 450 nm the focus is on minimising the loss. First consider the graph of figure 13. This is similar to the one in figure 12. Only this time the radius is varied rather than the width. What we observe from Figure 13 is that the radius already has its optimal value for r = 84nm. With this value for the mirror radius, losses are minimised.

Following the same procedure by varying the separation of the holes results in the graph shown in figure 14. The graph shows that the reflection is at its best when the centre to centre distance has a value of d = 303nm. Admittedly a decrease of the order 10^{-4} in loss is not very significant. On the other hand the minimum is just 1% off from the 300 nm. It turns out that we already were very close to the minimum.

This concludes the optimisation of the mirror. Yet in Subsection 4.3 we mentioned that adding more holes to the mirror will certainly improve reflection. The reason that we limited the mirror size in the first place was due to simulation time. However if one does have the time or the tools to run at higher resolutions, there will be room for improvement.

4.7 Results

With all the structural components at their optimal size, we have the structure we set out to find. Altogether the waveguide produces a band-gap with



Figure 13: The centre gap wavelength as a function of the radius of the holes in addition to the corresponding loss shown on the right vertical axis.



Figure 14: The centre gap wavelength as a function of the separation of the holes in addition to the corresponding loss shown on the right vertical axis.

its structure shown in figure 15. The final dimensions of design can be found in Table 2 in addition to some property values of the associated band-gap. Note that the centre gap wavelength is not at 782 nm while we set out to find it at 780 nm. This however does not result in a significant loss. The Difference in loss is about 10^{-4} . Even at wavelengths between 776 nm to 788 nm the loss is less than 10^{-3} higher that the minimum loss. This is why we are not concerned by the 2 nm deviation.



Figure 15: The band gap structure of the final dielectric waveguide mirror.

Before concluding this section, there are still some matters that need to be attended. Returning to Figure 13 of the last subsection, two points in the graph seem to deviate from the rest. At the radius of 85 nm the wavelength is about 1 nm higher than expected. yet one can hardly consider this as a deviation once the width of the band-gap is considered. The width is simply to broad for this to matter. Similarly at a radius of 88 nm the Loss is 10^{-4} lower then expected. This is once again an insignificant deviation and its relatively far from the radius of the minimum. Same arguments apply to the deviation point of Figure 14.

A second notable feature of Figure 13 is the relation of the radius size with the wavelength. In this graph the wavelength only has a range of 4.5 nm. Its too short to say anything conclusive about the actual relationship. Yet there is no denying that the wavelength is decreasing as the radius gets

Width waveguide	450 nm
Height waveguide	200 nm
Mirror size	7 holes
Mirror radius	84 nm
Mirror separation	303 nm
Taper size	7 holes
Taper radius	66 to 84 nm
Taper separation	257 to 300 nm
Centre-gap wavelength	782 nm
Loss at centre-gap	2.71×10^{-3}

 Table 2: The structural dimensions of the final the dielectric waveguide mirror.

larger. This does agree with the statement made earlier about effective index of the waveguide. So does the increasing of the wavelength with increasing separation as shown in Figure 14. It seems that the wavelength of the band gap indeed increases as the effective index of the waveguide gets larger.

We set out to find the mirror made out of a silicon nitride waveguide with its height not larger than 200 nm and its band gap centred at 780 nm wavelength. The structure given by Table 2 satisfies these requirements. Moreover, a comparison between the graph of figure 15 and that of figure 10 shows that we successfully relocated the band gap while keeping the loss at the same order of magnitude. This means that a cavity can be constructed using these mirrors. However one may need to use a larger size mirror to get a higher Q-factor for the cavity. This should not change the centre gap wavelength significantly as indicated by a comparison between the graph of Figure 9 and that of Figure 10. This comparison also shows that the shape of the band gap does not change significantly close to the centre of the gap. Considering the width of the gap close to its centre, one does not need to concern oneself with a deviations of several nm from this centre.

5 reference

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